

## **Thermo-acoustical and non-linear molecular interaction studies in ternary liquid mixtures at 298K**

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**ABSTRACT:** *The ultrasonic studies in liquids are great use in understanding the nature and strength of molecular interaction. The thermo-acoustical parameters for ternary liquids mixtures namely, Chlorobenzene + Benzene +Tetrahydrofuran (THF) have been estimated, from the measured values of ultrasonic velocity (U), density ( $\rho$ ) and viscosity ( $\eta$ ). For velocity measurement, Ultrasonic Interferometer was used with an accuracy of  $\pm 0.01\text{ms}^{-1}$  working at fixed frequency 3MHz. The density of pure liquids and liquid mixtures was determined using pycnometer by relative measurement method with an accuracy of  $\pm 0.1\text{Kgm}^{-3}$ . An Ostwald's viscometer was used for the viscosity measurement of pure liquids and liquid mixtures with an accuracy of  $\pm 0.0001\text{NSm}^{-2}$ . Using the measured data, some of the acoustical parameters such as, adiabatic compressibility ( $\beta_a$ ), free length ( $L_p$ ), free volume ( $V_p$ ), internal pressure ( $\pi_i$ ), relaxation time ( $\tau$ ), and Gibb's free energy ( $\Delta G$ ) are evaluated at the temperature 298K. The present paper represents the nonlinear variation of ultrasonic velocity and the thermo-acoustical parameters lead to dipole- induced dipole interaction between chlorobenzene and benzene molecule while dipole-dipole interaction between the chlorobenzene and THF molecule. The behavior of these parameters with composition of the mixture has been discussed in terms of molecular interaction between the components of the liquids.*

**Keywords:** *Ultrasonic velocity, acoustical parameters, molecular interactions, Chlorobenzene, Benzene, Tetrahydrofuran (THF) and ternary mixtures.*

### **I. INTRODUCTION**

Ultrasonic study is very much useful for characterizing the physico-chemical behavior of liquids mixtures and measurements are used to study molecular interactions in the liquids [1, 2]. The method of studying in molecular interaction from the knowledge of variation of acoustic parameters values with change in mole fraction gives an insight into the molecular process [3, 4]. The increase or decreases in ultrasonic velocities have been employed in understanding the nature of molecular interaction in the pure liquids binary mixtures [5-8] and ternary mixtures [9, 10]. The study of liquid mixtures containing of polar and non-polar components find applications in industrial and technological process [11]. The mixing of different components gives rise to solutions that generally do not behave ideally [12, 13]. Further these properties have been widely used to study the molecular interaction between the various species in the mixture [14, 15].

In present study ultrasonic velocity, density and viscosity were measured experimentally for the ternary systems namely Chlorobenzene + Benzene + Tetrahydrofuran at 298K. From the measured data, thermo-acoustical parameters have been computed and the results are analyzed in the light of molecular interaction.

### **II. EXPERIMENTAL DETAILS:**

The liquid mixtures of various concentrations in mole fraction were prepared by taking AR grade chemicals. In the ternary mixture system, the mole fraction of second component, Benzene ( $X_2$ ) is kept fixed arbitrarily at  $X_2 = 0.40$ . Mole fraction of Chlorobenzene ( $X_1$ ) is increased from 0.00 to 0.60 while mole fraction of THF ( $X_3$ ) is decreased from 0.60 to 0.00. The ultrasonic velocity in the liquid mixtures have been measured using an ultrasonic interferometer (Mittal type: Model: M-83) working at frequency 3MHz with an overall accuracy of  $\pm 0.1\text{ms}^{-1}$ . An electronically digital operated constant temperature water bath has been used to circulate water through the double walled measuring cell made up of a steel containing the experimental solution at the desired temperature. The density of pure liquids and liquid mixtures was determined using 25ml specific gravity bottle with an accuracy of  $\pm 0.1\text{Kgm}^{-3}$ . An Ostwald's viscometer was used for the viscosity measurement of pure liquids and liquid mixtures with accuracy  $0.0001\text{Nm}^{-2}\text{s}$ . The viscometer was calibrated before used. The time of flow of water ( $t_w$ ) and time flow of solution ( $t_s$ ) was measured with digital stop watch. All the precautions were taken to minimize the possible experimental error.

### **III. RESULTS AND DISCUSSION:**

Adiabatic compressibility ( $\beta_a$ ) have been calculated from the ultrasonic velocity (U) and the density ( $\rho$ ) of the medium using the equation as:

$$\beta_a = 1 / U^2 \rho \quad \dots\dots\dots (1)$$

Intermolecular free length has been determined as:

$$L_f = K_T (\beta_a)^{1/2} \quad \dots\dots\dots (2)$$

Where  $K_T$  – is a Jacobson’s constant.

Free volume in terms of ultrasonic velocity (U) and viscosity of the liquid ( $\eta$ ) as :

$$V_f = [ M_{eff} U / K \eta ]^{3/2} \quad \dots\dots\dots (3)$$

Where- $M_{eff}$  is the effective molecular weight ( $M_{eff} = \sum m_i X_i$ , in which  $m_i$  and  $X_i$  are the molecular weights and the mole fraction of the individual constituents respectively).  $K$  is a temperature independent constant which is equal to  $4.28 \times 10^9$  for all liquids.

Internal pressure is calculated by

$$\Pi_i = bRT (K \eta / U)^{1/2} (\rho^{2/3} / M^{7/6}) \quad \dots\dots\dots (4)$$

Where,  $b$  stands for cubic packing which is assumed to be 2 for all liquids and  $K$  is a dimension less constant, independent of temperature and the nature of liquids and its value is  $4.28 \times 10^9$ ,  $T$  is the absolute temperature and  $M_{eff}$  is the effective molecular weight.

Relaxation time in terms of adiabatic compressibility ( $\beta_a$ ) and viscosity of the liquid ( $\eta$ ) as:

$$\tau = 4/3 \beta_a \eta \quad \dots\dots\dots (5)$$

Gibb’s free energy can be calculated from the following relation:

$$\Delta G = KT \log (KT\tau / h) \quad \dots\dots\dots (6)$$

Where,  $\tau$  is the relaxation time,  $K$  the Boltzmann constant,  $T$  the absolute temperature and  $h$  is the Planks constant.

The experimental data relating to density, viscosity and ultrasonic velocity at 298K for frequency 3MHz of the mixtures are given in Table-1. The calculated values of adiabatic compressibility ( $\beta_a$ ), free length ( $L_f$ ) and free volume ( $V_f$ ) are reported in Table-2. Internal pressure ( $\pi_i$ ), viscous relaxation time ( $\tau$ ) and Gibb’s free energy ( $\Delta G$ ) are reported in Table-3.

From the Table- 1, it is observed that, the density ( $\rho$ ) and viscosity ( $\eta$ ) increases with increase in concentration of chlorobenzene and ultrasonic velocity decreases with increase. The decreases in ultrasonic velocities are due to the decrease in adiabatic compressibility and free length of the liquid mixtures. This may lead to the presence of dispersive force (London force) between the molecules of the liquid mixture [16]. The adiabatic compressibility and intermolecular free length are the deciding factors of ultrasonic velocity in the ternary liquid mixtures. The decrease in free volume (Table- 2) and increase in internal pressure (Table- 3) represent that, the strength of the interaction decreases with the increase in solute concentration. It also represents that there is weak interaction between the solute and solvent molecules [17].

The relaxation time (Table- 3) increases with increase in concentration of Chlorobenzene, which is in the order of  $10^{-12}$ sec., is due to structural relaxation process [18] and in such a situation, it is suggested that, the molecule gets rearranged due to co-operative process. From the Table- 3, the Gibb’s free energy ( $\Delta G$ ) increases with increase in concentration chlorobenzene, which may due to intermediate compound formation between the ternary liquid mixtures.

As benzene is non- polar molecule doesn’t possess dipole moment, when it interacts with chlorobenzene which is polar molecule possess dipole moment then benzene possess induced dipole moment. This is the induced dipole - dipole interaction between benzene and chlorobenzene molecule. Also there is dipole – dipole interaction between the chlorobenzene and Tetrahydrofuran molecule. Hence there exists dipole-dipole interaction between the chlorobenzene and Tetrahydrofuran molecule and dipole – induced dipole interaction between chlorobenzene- benzene molecules.

#### IV. FIGURES AND TABLES

TABLE 1: The experimental values of adiabatic compressibility ( $\beta_a$ ), free length ( $L_f$ ) and free volum ( $V_f$ ) for the ternary system- Chlorobenzene + Benzene + Tetrahydrofuran at 298K.

Mole fraction		Compressibility ( $\beta_a$ ) ( $10^{-10} \text{ m}^2 \text{ N}^{-1}$ )	Free length ( $L_f$ ) ( $10^{-10} \text{ m}$ )	Free volume ( $V_f$ ) ( $10^{-7} \text{ m}^3 \text{ mol}^{-1}$ )
$X_1$	$X_3$			
0.0000	0.6000	8.378	0.5731	3.2811
0.1000	0.5000	7.057	0.5261	2.3507
0.1999	0.4001	7.099	0.5275	2.4614
0.2999	0.3001	7.057	0.5261	2.3180
0.4000	0.2000	6.848	0.5181	2.2859
0.5001	0.0999	6.976	0.5229	2.3639

0.6000	0.0000	7.061	0.5261	2.4183
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adiabatic compressibility( $\beta_a$ ), free length ( $L_f$ ), free volume( $V_f$ ), internal pressure( $\pi_i$ ), relaxation time( $\tau$ ), and Gibb's free energy( $\Delta G$ ) with respect to mole fraction at temperature 298K.

## V. CONCLUSION

From ultrasonic velocity, related acoustic parameters for ternary mixtures of chlorobenzene with Tetrahydrofuran in benzene for various concentration at 298K, it has been found that there exists a dipole-induced dipole interaction between chlorobenzene and benzene while dipole-dipole interaction between the chlorobenzene and Tetrahydrofuran molecule.

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